ARCHER and ARCHER2 Quarterly Report

October – December 2020

EPCC

The University of Edinburgh

epcc

1. Document Information and Version History

Version:	1.0
Status	Release
Author(s):	Lorna Smith, Juan Rodriguez Herrera, Chris Johnson, Xu Guo, George Beckett
Reviewer(s)	Alan Simpson

Version	Date	Comments, Changes, Status	Authors, contributors, reviewers
0.1	2021-01-15	Initial draft	Lorna Smith
0.2	2021-01-27	Content added by team leaders	Juan Rodriguez Herrera, Chris Johnson, Xu Guo, George Beckett
0.3	2021-01-27	First full draft created	Lorna Smith
0.4	2021-01-28	Reviewed	Alan Simpson
1.0	2021-01-28	Version for UKRI	Alan Simpson, Lorna Smith

ARCHER Quarterly Report

This section of the report covers the period October 2020, November 2020 and December 2020 for the ARCHER2 service.

2. ARCHER Executive Summary

- The ARCHER service closed on Wednesday the 27th January at 8am after 7 years of service.
- Any remaining CSE queries will transfer to ARCHER2, if appropriate.

3. ARCHER Forward Look

- The ARCHER service has now closed and future efforts will focus on the ARCHER2 service.

4. ARCHER Performance Report

This is the performance report for ARCHER CSE Service for the Reporting Periods: October 2020, November 2020 and December 2020.

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER CSE Service Contract.

CSE Query Metrics

- **QE1:** The percentage of all queries notified to the Contractor by the Help Desk in a Quarter that the Contractor responds to, and agrees a work plan with, the relevant End User within 3 working hours of receiving the notification from the Help Desk. *Service Threshold: 97%; Operating Service Level: 98%.*
- **QE2:** The percentage of all queries notified by the Help Desk to the Contractor that have been satisfactorily resolved or otherwise completed by the Contractor within a 4-month period from the date it was first notified to the Contractor. *Service Threshold: 80%; Operating Service Level: 90%.*
- **TA1:** The percentage of all technical assessments of software proposals provided to the Contractor by the Help Desk in any Service Period that are successfully completed by the Contractor within 10 days of the technical assessment being provided to the Contractor by the Help Desk. *Service Threshold: 85%; Operating Service Level: 90%.*
- **FB1:** The percentage of End User satisfaction surveys for CSE queries carried out in accordance with the Performance Monitoring System by the Contractor showing the level of End User satisfaction to be "satisfactory", "good" or "excellent". *Service Threshold: 30%; Operating Service Level: 50%.*

Period	October 2020		November 2020		December 2020		Q4 2020	
Metric	Perf	SP	Perf	SP	Perf	SP	Perf	Total
QE1	100%	-2	100%	-2	-		100%	-4
QE2	100%	-2	100%	-2	100%	-2	100%	-6
TA1	100%	-1	-		-		100%	-1
FB1	100%	-2	-		100%	-2	100%	-4
Total		-7		-4		-4		-15

Service Credits

Period	October 2020	November 2020	December 2020
Total Service Points	-7	-4	-4

5. ARCHER CSE Queries

This section provides details on ARCHER CSE queries during the period October –December 2020.

Queries Resolved in Reporting Period

Metric Descriptions

In-Depth	All technical queries passed to ARCHER CSE team
Technical Assessment: <Category>	Request for Technical Assessments of applications for ARCHER time
Course Enquiry	Enquiries about courses

A total of 18 queries were resolved by the CSE service in the reporting period.

Metric	October-20	November-20	December-20	Total
In-depth	7	2	6	15
Technical Assessment: Instant	1	0	0	1
Course Enquiry	0	0	2	2
Total	8	2	8	18

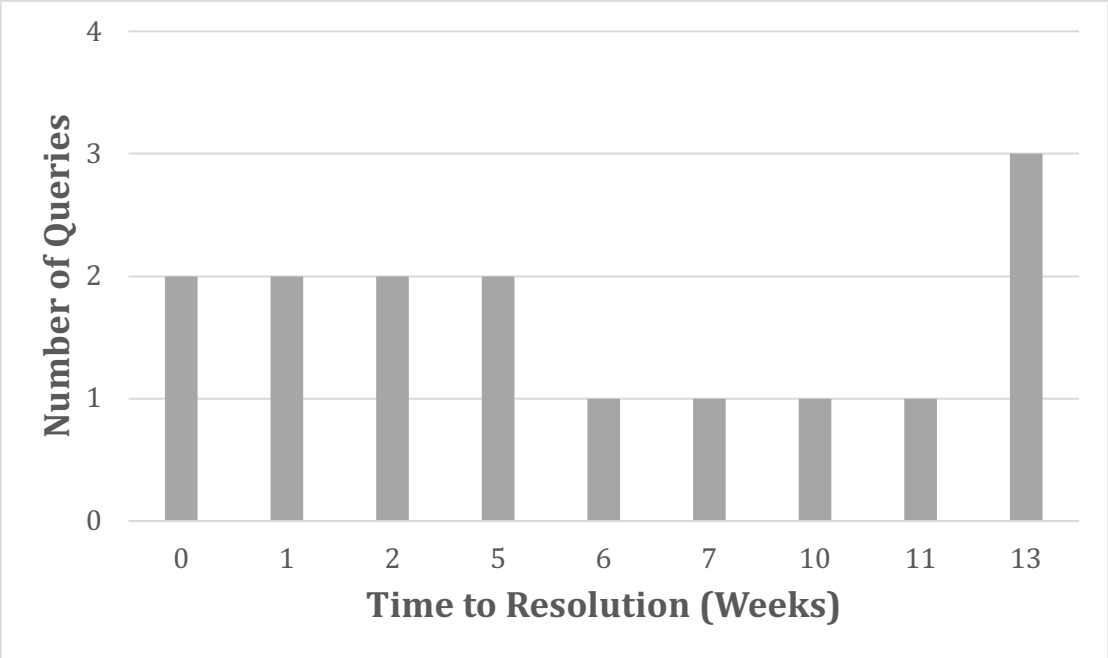
3 query feedback responses were received on In-depth queries in the reporting period. Two responses a score of “Excellent” and one of “Good”.

Resolved In-Depth queries fell into the following categories:

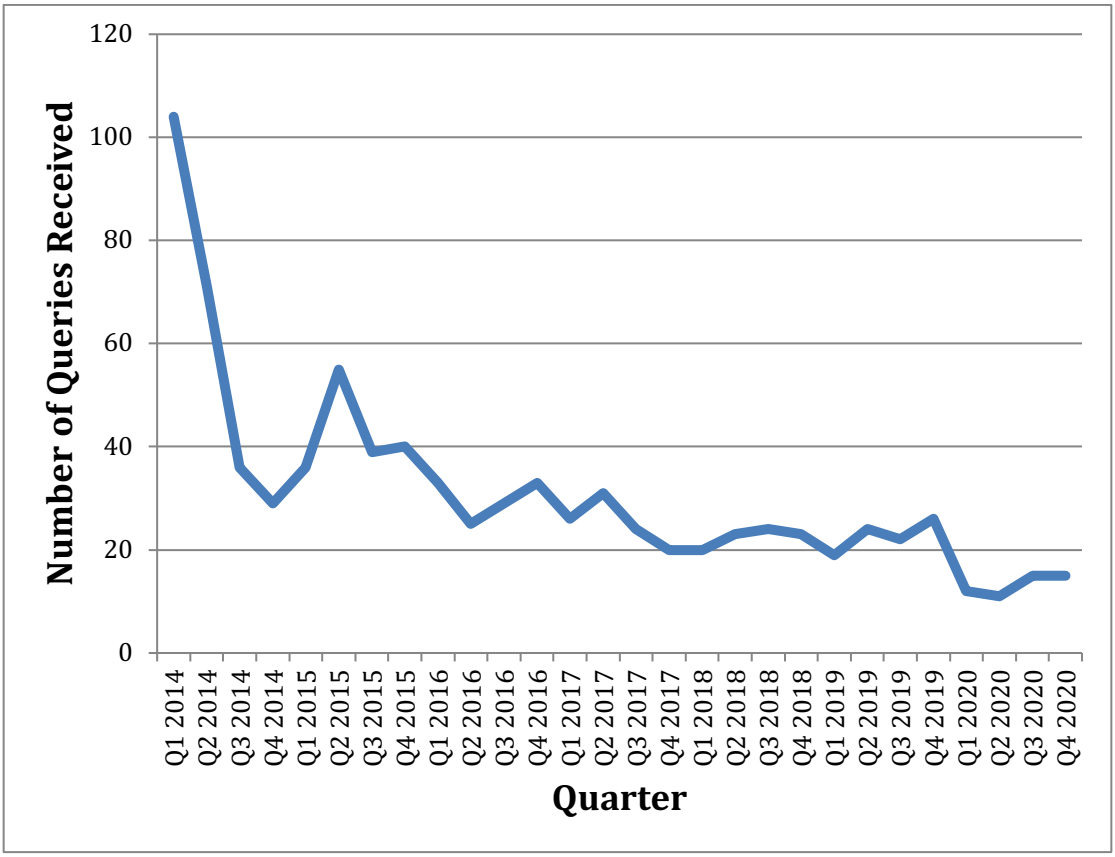
Category	Number of Queries	% Queries
3rd party software	10	66.7%
User programs	2	13.3%
Login, password and ssh	2	13.3%
Batch system and queues	1	6.7%

In-depth Query Analysis

The histogram below shows the time to resolution for In-Depth queries in the current reporting period.

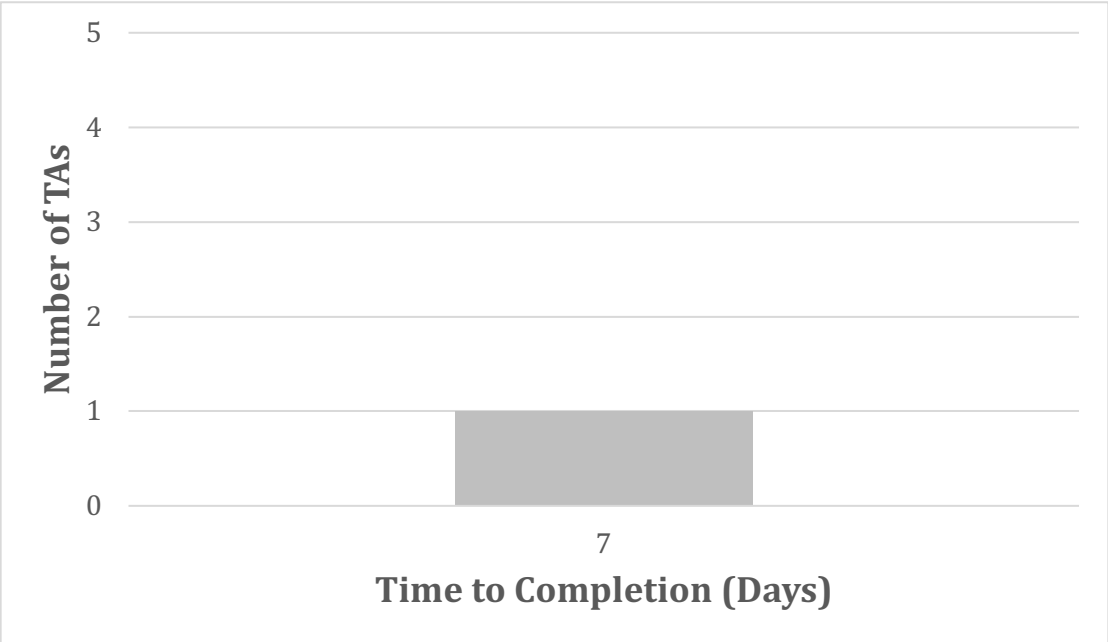


Plot of numbers of ARCHER In-Depth queries received per quarter:

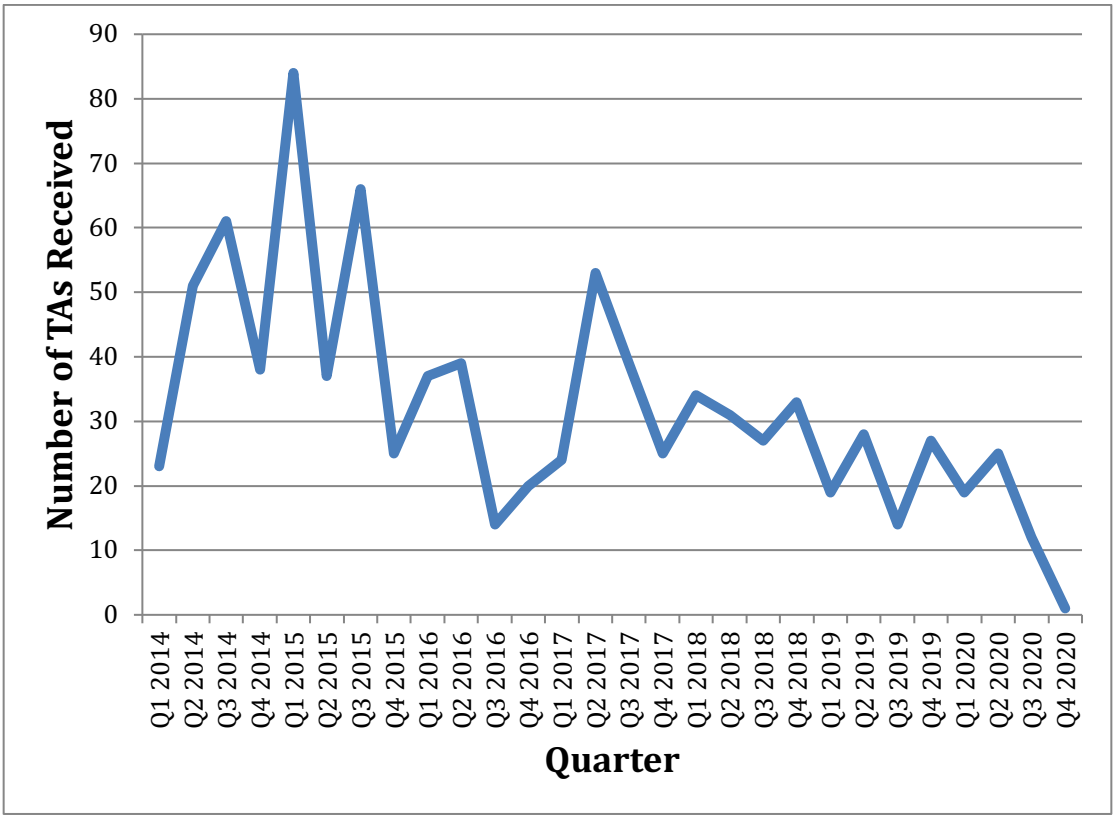


Technical Assessment Analysis

A histogram of the time to completion for ARCHER Technical Assessments is shown below.



Plot of numbers of ARCHER Technical Assessments received per quarter:



ARCHER 2 Quarterly Report

This section of the report covers the period October 2020, November 2020 and December 2020 for the ARCHER2 service.

6. ARCHER2 Executive Summary

- The CSE team have engaged with the early-access programme to complete preparations for ARCHER2 early-life support. Documentation and tools have been developed to support the migration of users' data from ARCHER to ARCHER2.

- We have continued to provide in-depth support for ARCHER users, to ensure continued science-productivity during preparations for the transition to ARCHER2.

- A total of 18 days of training days, which comprises 10 courses and 4 virtual tutorials, have taken place in this quarter. All courses were delivered online.

- Just after the ARCHER2 4 cabinet system was open to a set of early-access users, several runs of introductory courses to ARCHER2 took place: two courses aimed for software package users, and two for software developers. This material was developed rapidly once access was provided to the early-access pilot system at the HPE Cray factory in the USA. These courses have been well received and provided early experience to our user community.

- Three eCSE calls have successfully been issued during the first year of ARCHER2; the first two received a total of 37 proposals with 20 projects being awarded a total of 185 Person Months. The third call is presently open, closing on 16 March 2021.

- A call for Early Career Observers was launched alongside the 2nd eCSE call with 5 people accepted by the eCSE Panel. This has provided early-career researchers with experience of the workings of peer-reviewed panels. Feedback from these Observers has been positive.

- The CSE team collaborated on running two sessions at the Supercomputing Conference (SC20) in November, focused towards online HPC education. A key focus was on ensuring that online training is as inclusive, accessible and engaging as possible, regardless of the student background.

- We also took key roles in the HPC Champions online event in December, giving presentations and leading discussion sessions. The event was again well attended.

7. ARCHER2 Forward Look

- During this next period: the ARCHER service is switched off; the 4 cabinet system operates as the sole platform for our user community; and the 19 cabinet system arrives on site.

- Our primary focus will be on supporting users as they utilise the 4 cabinet system as they port, run and optimise their application codes on this new system. We will also prepare for the transition to the 19 (and 23) cabinet system when it comes online.

- Two new courses, entitled "Understanding Package Performance" and "Performance Optimisation on AMD EPYC", will be delivered in January. After opening the ARCHER2 4-cab system for all users, these courses will target important concepts such as performance and code optimisation on ARCHER2.

- A new package-specific course, Code_Saturne, will be offered in March. This package is centrally installed on ARCHER2 and users will benefit from having a course delivered by the main code developers.

- Plans are underway to offer "lightweight" eCSE project requiring between 1-3 PMs of effort to bridge the gap between in-depth queries (up to 35 days) and regular eCSE (between 3-12 PMs). Discussions with the eCSE panel as to how to offer this are underway.

- Alongside the "lightweight" eCSE, we are investigating ways in which to encourage proposals from researchers earlier on in their careers than those who are presently most likely to apply.

8. ARCHER2 Centralised CSE Team

During the period, the CSE team focused on preparing the ARCHER2 4-cabinet service for early operations.

They played a key role in service-validation activities, intended to inform the timeline for closing ARCHER and moving to ARCHER2, including:

- measuring the performance, reliability, and code-reproducibility characteristics of the 4-cabinet system
- validating key scientific application and libraries
- developing good practice for using the batch system, programming environments, and containerised workflow support.

An early-access programme ran for much of the period (beginning on 21st October) with selected, experience computational scientists from EPRSC and NERC high-end consortia being given access to ARCHER2, to test and optimise their key science use cases and workflows. The CSE team worked closely with the early-access-programme members and, with their help, were able to identify and resolve/ work around a number of early-life snags, such that, by the end of December, almost all of the key science use cases had been successfully demonstrated on the 4-cabinet system.

Alongside work on ARCHER2, the CSE team also helped users prepare for the end of the ARCHER service, with a focus on data-migration requirements. The CSE team produced good-practice documentation to help users migrate their necessary data from ARCHER to ARCHER2, included written notes, video demonstrations, and online webinars. The CSE team also tested and documented a streamlined, higher-bandwidth connection between ARCHER and ARCHER2 that was set up by SP, to support a rapid migration of users.

The team also continued to provide a full programme of science support to ARCHER users, ensuring users could continue with their research programmes (including priority access for Covid-19-related research), during preparations for ARCHER2, and in spite of challenges associated with the pandemic.

CSI Projects

The CSE team also made progress with several, early-life service-improvement projects, as follows:

- *Software-management package evaluation.* The team completed an evaluation of two software-management packages, called EasyBuild and Spack, which each had the potential to streamline and enhance the deployment of centrally managed software packages. The evaluation concluded that Spack was a promising tool for software management on ARCHER2, but that further work would be needed, from the Spack development team, to accommodate specific aspects of the HPE Cray EX platform. Work has been paused, though we anticipate proceeding with a Spack deployment early on in the life of the full (23-cabinet) ARCHER2 service.
- *Software logging tools.* The team began work to set up the software logging tool X-Alt on the 4-cabinet system. X-Alt had previously been used successfully on ARCHER to monitor usage of centrally installed software and packages, and to inform decisions about prioritisation of software upgrades and support. Recently, a new version of X-Alt has been developed (Version 2), which should mean a simpler and easier-to-manage deployment on ARCHER2. Work is on-going to evaluate X-Alt Version 2, with the aim of having the tool in production for the beginning of the full ARCHER2 service.

9. ARCHER2 Performance Report

This is the performance report for the ARCHER2 CSE Service for the Reporting Periods October 2020, November 2020 and December 2020. The metrics were specified by EPSRC in Schedule 2.2 of ARCHER2 CSE Service Contract.

CSE Query Metrics

- **ARCHER2_CSE_Level1 (MTR)**: The Median Time to Resolution, as measured by Working Days (WDs), of all CSE queries falling within Level 1 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >4.4 WD; Operating Service Level: >1.4 WD, ≤2.4 WD.*
- **ARCHER2_CSE_Level2 (MTR)**: The Median Time to Resolution, as measured by Working Days (WD), of all CSE queries falling within Level 2 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >27 Working Days (WD); Operating Service Level: >12 WD, ≤17 WD.*
- **ARCHER2_CSE_Level3 (MTR)**: The Median Time to Resolution, as measured by Working Days (WD), of all CSE queries falling within Level 3 resolved by the Contractor in the Reporting Period. *Initial MTR applicable to OY1: Service Threshold: >59 Working Days (WD); Operating Service Level: >29 WD, ≤39 WD.*
- **ARCHER2_CSE_TA (%):** The percentage of the total number of Technical Assessments (TAs) assigned to the Contractor in the Reporting Period completed prior to the commencement of the applicable TA Target Completion Date after the assignment of such Technical Assessment to the Contractor. *TA Target Completion Date in OY1: 8 WD; Service Threshold: <90.00%; Operating Service Level: 95.00-97.49%.*
- **Initial Response to Queries (%):** The percentage of the total number of CSE queries assigned to the Contractor in the Reporting Period responded to within 3 Working Hours. *Service Threshold: <96.00%; Operating Service Level: 98.00 – 98.99%.*
- **Query User Satisfaction (%):** The percentage of the total number of query satisfaction surveys completed in each Reporting Period, rating the quality of the resolution of Queries by the Contractor as "Good", "Very Good" or "Excellent". *Operating Service Level: 82.00 – 87.99%.*
- **Training User Satisfaction (%):** The percentage of all training satisfaction surveys completed in each Service Period, rating the Contractor as "Good", "Very Good" or "Excellent". *Operating Service Level: 88.00%-92.99%.*

Metric	Oct-2020		Nov-2020		Dec-2020		Q4 2020	
	Perf	Points	Perf	Points	Perf	Points	Perf	Points
ARCHER2_CSE_Level1 (MTR)	0.1 WD	-2	0.1 WD	-2	0.1 WD	-2	0.1 WD	-6
ARCHER2_CSE_Level2 (MTR)	0.9 WD	-2	0.4 WD	-2	0.1 WD	-2	0.4 WD	-6
ARCHER2_CSE_Level3 (MTR)	-		-	-	10.5 WD	-2	10.5 WD	-2
ARCHER2_CSE_TA (%)	100%	-1	100%	-1	100%	-1	100%	-3
Initial Response to Queries (%)	99.7%	-0.25	100%	-1	100%	-1	99.8%	-2.25
Query User Satisfaction (%)	100%	-2	100%	-2	100%	-2	100%	-6
Training Satisfaction (%)	95.6%	-0.25	90.9%	0	100%	-1	96.6%	-1.25
Total		-7.5		-8		-11		-26.5

97 query feedback responses were received on query resolution in the Reporting Period. 100% of responses had a score of "Good", "Very Good" or "Excellent".

59 training satisfaction responses were received in the Reporting Period. 96.6% of responses had a score of "Good", "Very Good" or Excellent". There were two "Bad" responses.

10. ARCHER2 CSE Queries

This section provides details on ARCHER2 CSE queries during the Reporting Period October – December 2020.

CSE Query Statistics

The metrics were specified by EPSRC in Schedule 2.2 of ARCHER2 CSE Service Contract.

- **No. of Assigned:** The number of CSE queries assigned to the Contractor within each query resolution category in the Reporting Period.
- **No. of Resolved:** The number of CSE queries resolved by the Contractor within each query resolution category in the Reporting Period.
- **Backlog:** The number of CSE queries assigned to the Contractor that remained unsolved within each query resolution category in the Reporting Period
- **Avg No. of Correspondence:** The average number of pieces of correspondence generated for CSE queries in each query resolution category.
- **Avg Time of First Responses:** The average time taken for the Contractor to first respond to the Originator of the CSE query.

A total of 581 queries were resolved by the ARCHER2 CSE service in the Reporting Period.

October 2020					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	252	256	1	4	0.3 hrs
ARCHER2_CSE_Level2	45	44	6	11	0.3 hrs
ARCHER2_CSE_Level3	1	0	0	-	-
ARCHER2_CSE_TA	7	5	1	19	2.8 hrs
November 2020					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	112	112	1	4	0.5 hrs
ARCHER2_CSE_Level2	28	22	12	14	0.3 hrs
ARCHER2_CSE_Level3	3	0	4	-	-
ARCHER2_CSE_TA	4	7	0	14	1.2 hrs
December 2020					
Service level	**Assigned**	**Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	110	111	0	4	0.6 hrs
ARCHER2_CSE_Level2	8	15	5	10	0.3 hrs
ARCHER2_CSE_Level3	5	1	8	59	0.2 hrs
ARCHER2_CSE_TA	9	8	2	13	0.5 hrs
Q4 2020					
Service level	**No. of Assigned**	**No. of Resolved**	**Backlog**	**Average Correspondence**	**Average Time First Response**
ARCHER2_CSE_Level1	474	479	0	34	0.4 hrs
ARCHER2_CSE_Level2	81	81	5	12	0.3 hrs

ARCHER2_CSE_Level3	9	1	8	59	0.2 hrs
ARCHER2_CSE_TA	20	20	2	14	1.3 hrs

CSE Query Categories

Resolved CSE queries in the Reporting Period fell into the following categories:

Service Level	Category	Number of Queries	% Queries
ARCHER2_CSE_Level1	Course registration	454	78.1%
	Training enquiries	24	4.1%
	Call-backs	1	0.2%
ARCHER2_CSE_Level2	eCSE applications/calls	29	5.0%
	3rd party software	22	3.8%
	Batch system and queue	12	2.1%
	Compilers and system software	6	1.0%
	Access to HPC	3	0.5%
	User programs	2	0.3%
	Training enquiries	2	0.3%
	SAFE	1	0.2%
	Login, password and ssh	1	0.2%
	Performance and scaling	1	0.2%
	Data transfer	1	0.2%
	Other	1	0.2%
ARCHER2_CSE_Level3	3rd party software	1	0.2%
ARCHER2_CSE_TA	EPSRC Grant	19	3.3%
	Pioneer Projects	1	0.2%
Total		581	100.0%

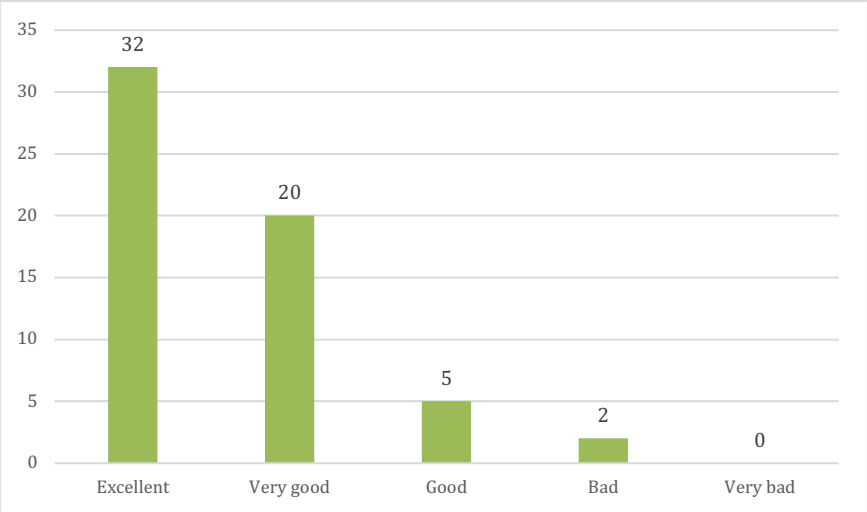
11. ARCHER2 Training

As part of ARCHER2, the service has been developing and delivering online a training programme for the ARCHER2 community. During the last quarter of 2020, the CSE service has provided a total of 18 days of online training, scheduled as follows:

Dates	Course	Days	Attendees
6, 8, 13, 15 Oct 2020	Shared-memory programming with OpenMP	2	24
13, 20 Oct 2020	Practical introduction to QM/MM using CP2K for biomolecular modelling	1	26
14 Oct 2020	Differences between ARCHER and ARCHER2	0.5	68
19-22 Oct 2020	Data Carpentry	2	10
21 Oct 2020	Slurm scheduling system on ARCHER2	0.5	36
28 Oct 2020	Access mechanisms for ARCHER2	0.5	33
28-29 Oct 2020	ARCHER2 for software developers	2	18
30 Oct 2020	ARCHER2 for software package users	1	4
2-5 Nov 2020	Software Carpentry	2	17
11 Nov 2020	Data Analytics using Python	1	20
18 Nov 2020	Exploring the binding site of the SARS-CoV-2 main protease using HPC	0.5	50
8-9 Dec 2020	Reproducible computational environments using containers - Introduction to Docker and Singularity	2	25
10 Dec 2020	ARCHER2 for software package users	1	10
14-15 Dec 2020	ARCHER2 for software developers	2	9

The above table lists a total of 10 courses, where three of them were new, and 4 virtual tutorials. Several runs of the brand-new introductory courses to ARCHER2 have taken place since the ARCHER2 4-cab system was open for early access: two courses aimed for software package users, and two for software developers. The development of these courses started once EPCC had access for the first time to the early-access pilot system at the HPE Cray factory in the USA.

On the feedback for online courses, attendees rate the course on a scale of 1-5 (“Very Bad”, “Bad”, “Good”, “Very Good” and “Excellent”). The average feedback using this metric was 4.4, i.e., better than “Very Good”. Users provided 59 feedback forms, a response rate of 36%.



12. ARCHER2 The Embedded CSE Programme (eCSE)

As part of ARCHER2, the CSE service will deliver an eCSE programme to provide distributed CSE support across the UK. The service will deliver an average of 12 FTEs over its lifetime. In order to enhance support for researchers in the early stages of their careers, we are offering the opportunity for a small number of early career researchers to attend the eCSE panel meeting as observers. The first batch of successful candidates attended the second eCSE panel meeting.

The 1st ARCHER2 eCSE call

- The first eCSE call opened for codes within the EPSRC remit on 19 May 2020 and closed on 7 Jul 2020. This call received 25 proposals from a broad range of subject areas within the EPSRC remit, with PIs from 15 different UK Institutions. Overall a total of 235 Person-Months of effort was requested from 13 different UK institutions.
- From this call 13 projects were awarded a total of 132 PMs overall. Projects have either started or will start during the next quarter.

The 2nd ARCHER2 eCSE call

- The second eCSE call opened on 8 Sep 2020 and closed on 27 Oct 2020 initially receiving 13 technical evaluations of which 12 became full proposals from 11 different UK institutions. Overall a total of 107 PMs of effort were requested from 11 different UK institutions. This call was open to applications within both the EPSRC and NERC remit.
- From this call 7 projects were awarded a total of 53 PMs overall.
- Several enhancements to the application process and associated forms were made for this call to assist with both the application and review process. Projects have either started or will start during the next two quarters.

The 3rd ARCHER eCSE call

- The third eCSE call opened on 8 Dec 2020.
- Given the restrictions many are finding due to the increased COVID lockdown, in particular school closures and the fact that restrictions affect different people in different ways, in early Jan 2021 the decision was taken to delay the deadlines for technical evaluations and full proposals by 4 weeks. The ARCHER2 Service is committed to equality, diversity, inclusion and accessibility and we believe that giving this extension will allow as many people to participate in the call as possible. The call will now close for technical evaluations on 23 Feb 2021 and for full proposals on 16 Mar 2021.

The 4th ARCHER eCSE call

- The 4th call is planned to open on 20 Apr 2021, closing for technical evaluations on 28 May and for full proposals on 8 Jun 2021.
- We intend to open the call up to proposals for shorter projects (less than 3 PMs). Discussion has begun with the Panel on how to run such a “lightweight” call in order to maximise the benefit to applicants.

Early Career Observers call

- The Early Career Observers call opened together with the second eCSE call on 8 Sep 2020 with the same deadline as the eCSE technical evaluation (6 Oct 2020).
- The call received 7 proposals which were assessed by three members of the eCSE Panel. Of the proposals, 5 candidates were chosen who all attended the panel meeting on 24 Nov 2021. These attendees agreed to the same conflicts of interest policies as regular panel members. Feedback from candidates was overwhelmingly good and clearly showed the experience had been positive for them.
- We plan to open a second observers call during 2021.

13. ARCHER2 Community Engagement, Outreach, Collaboration and Impact

In the past period, EPCC has focused its efforts towards better inclusivity and broader community diversity through teaching, training, and community building, leading several activities at the Supercomputing Conference, in November, as well as on-line via the HPC Certification Forum.

Weronika Filinger (ARCHER2 CSE) together with Julia Mullen (MIT Lawrence Livermore), Ann Backhaus (Pawsey) and Mozhgan Kabiri Chimeh (NVIDIA) presented two sessions at the Supercomputing Conference (SC20) in November, focused towards online HPC education. The first one was the State of the Practice Talk "Interactivity, engagement and community building in online HPC education and training", and the other was the Birds of a Feather session "Strategies for transitioning to Online HPC Education and Training". A key focus was on ensuring that online training is as inclusive, accessible and engaging as possible, regardless of the student background. Given the popularity of the two SC20 sessions the four presenters also organised a first session in a mini-series of workshops on "Building Effective Live sessions for Online Education". The cultural background of learners is one of the important elements to consider in planning and running engaging live sessions, and was one of the discussion topics.

Through the ACM SIGHPC Education Chapter and the International HPC Certification Forum, we organised a community-wide discussion, focused on schemes for making training content more searchable, accessible, navigable and identifiable – for both learners and educators. The motivation for doing this was to map between the skills defined by the HPC Certification Forum and existing training resources the group known to the group. The discussion was open to anyone interested in the subject: Many HPC educators from the USA and Europe attended.

EPCC and the ARCHER2 team have continued to steward Women in HPC, with Mark Parsons representing the Centre on the WHPC Steering Committee and George Beckett as treasurer for the organisation. Some elements of the usual WHPC programme have had to be re-scheduled/ adjusted in light of the Covid-19 pandemic, though we still had a visible presence at Supercomputing 2020 with our most successful WHPC workshop to-date, attracting in excess of 100 attendees. We also welcomed four new WHPC Chapters into the organisation, representing Australasia, Costa Rica, as well as two new chapters in the United States, bringing the chapter count to fifteen (https://womeninhpc.org/membership/chapters-and-affiliates/chapters).

Five of the ARCHER2 support team (David Henty, Juan Rodriguez Herrera, Lorna Smith, Jo Beech-Brandt, Julien Sindt) took part in the online HPC Champions event on the 15th December 2020. The meeting had a mix of invited speakers and discussion sessions and was well attended. Lorna Smith introduced the meeting, while Jo Beech-Brandt chaired the invited speaker session. David Henty led one of the discussion sessions around support for the installation of scientific software. There was also an interesting discussion topic around mentoring and diversity, and how this could be incorporated in to the eCSE programme.